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* * *	* *	* *	* *	* Welcome to STN International * * * * * * * * * *
NEWS	1			Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC	01	ChemPort single article sales feature unavailable
NEWS	3	APR	03	CAS coverage of exemplified prophetic substances
				enhanced
NEWS		APR		
NEWS	5	APR	24	
				information
NEWS	6	APR	26	USPATFULL and USPAT2 enhanced with patent
	_			assignment/reassignment information
NEWS		APR		CAS patent authority coverage expanded
NEWS		APR		ENCOMPLIT/ENCOMPLIT2 search fields enhanced
NEWS	9	APR	28	Limits doubled for structure searching in CAS
				REGISTRY
NEWS				
				STN on the Web enhanced
NEWS	12	MAY	11	BEILSTEIN substance information now available on
	4.0			STN Easy
NEWS	13	MAY	14	DGENE, PCTGEN and USGENE enhanced with increased
				limits for exact sequence match searches and introduction of free HIT display format
NEWS	2.4	1/2.1/	2.5	INPADOCDB and INPAFAMDB enhanced with Chinese legal
MEMS	14	PIAI	13	status data
NEWS	1.5	MAY	28	
MEMP	10	LIMI	20	records back to 1992
NEWS	16	.TIIN	0.1	CAS REGISTRY Source of Registration (SR) searching
HEND	10	0011	01	enhanced on STN
				cinaneca on our
NEWS	EXP	RESS	MAY	26 09 CURRENT WINDOWS VERSION IS V8.4,
				CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

Enter NEWS followed by the item number or name to see news on that specific topic.

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=> file registry COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.22 0.22

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 17 JUN 2009
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STRUCTURE FILE UPDATES: 15 JUN 2009 HIGHEST RN 1158168-92-3
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 $\label{thm:condition} $$ Uploading C:\Documents and Settings\vrodriguezgarcia\My Documents\e-Red Folder\10586573\Ll.str$

chain nodes:
7 8 9 10 11 13 14 15 16 17
ring nodes:
1 2 3 4 5 6 12 18 19 20 21 22
chain bonds:
6-7 7-8 7-11 8-9 9-10 10-15 11-12 11-13 13-14 13-16 16-17
ring bonds:
1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-22 18-19 19-20 20-21 21-22

exact/norm bonds:
7-11 8-9 9-10 10-15 13-14 13-16 16-17
exact bonds:
6-7 7-8 11-12 11-13
normalized bonds:
1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-22 18-19 19-20 20-21 21-22
isolated ring systems:
containing 1 : 12 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom

L1 STRUCTURE UPLOADED

=> s sam sss 11 SAMPLE SEARCH INITIATED 10:55:13 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 29 TO ITERATE

100.0% PROCESSED 29 ITERATIONS 4 ANSWERS SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
PROJECTED ITERATIONS: 257 TO 903
PROJECTED ANSWERS: 4 TO 200

L2 4 SEA SSS SAM L1

=> d sca

L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, a-[2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-ylloxyl-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, sodium salt (1:1)
MF C40 H38 F2 O10 S2. Na

Na

- L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- MF C40 H38 F2 O10 S2
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-[[[4,5-bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (\alpha Z)-MF C25 H28 N2 O13 S

- L2 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[1-[4-(aminosulfonyl)phenyl]-2-(benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI)$
- MF C24 H21 N O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> s full sss l1

100.0% PROCESSED

THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END;y FULL SEARCH INITIATED 11:12:39 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 767 TO ITERATE

SEARCH TIME: 00.00.01

84 ANSWERS

L3 84 SEA SSS FUL L1

=> d sca

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

767 ITERATIONS

- IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-
- MF C24 H28 F2 N O6 S
- CI COM

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (αZ)-MF C25 H30 O7 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, (<math>\alpha$ Z)-
- MF C29 H38 N2 O9 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]l-oxo-4-[((2Z)-1-oxo-2-propyloctyl]oxy]-2-buten-1-yl]oxy]-N,N,N-trimethylbromide (1:1)
- MF C33 H46 F2 N O6 S . Br

Absolute stereochemistry. Double bond geometry as shown.

• Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester,
- (αZ)-MF C24 H26 N2 O12 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (\alpha Z)-MF C25 H29 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acety)acy)-1-[4-(methy)sulfony])pheny][ethylidene]-4-fluoro-, 3-[4-[1-methyl-1-(nitrosothio)ethyl]-2-oxo-3-oxazolidinyl]propyl ester, (αZ) -
- MF C28 H31 F N2 O9 S2

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN L-Aspartic acid, 4-[(2Z)-3-(3,4-difluoropheny1)-4-ethoxy-2-[4-(methylsulfony1)pheny1]-4-oxo-2-buten-1-y1] ester
- MF C23 H23 F2 N O8 S

Absolute stereochemistry.
Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-,
- 3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester
- MF C36 H32 O10 S2
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-[[(4-bromobutoxy)carbony1]oxy]-1-[4-(methylsulfony1)pheny1]ethylidene]-, methyl ester, (αZ)-

MF C23 H25 Br 07 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(benzoyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI)
- MF C25 H22 O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
 IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-
- IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
- MF C24 H29 F N O6 S . Br

• Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (22)-2-[4-(methyleuifonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-oxo-3-phenyl-2-buten-1-yl ester
- MF C30 H38 N2 O11 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, a-[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, ethyl ester, (aZ)-
- MF C26 H31 N O10 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-4-[[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)carbonyl)oxy]-3-[4-(mthyloyl-2hydroyl)bhouyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N,N-krimethyl-1-2ng-2-bhts-1-ylloyl-N-krimethyl
- (methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-MF C36 H42 F2 N O8 S

Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, (α Z)-
- MF C25 H28 N2 O12 S

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α =[2-[[3-(bromomethy1)benzoy1]oxy]-1-[4-(methylsulfony1)phenyl]ethylidene]-, methyl ester, (αZ) -MF C26 H23 Br O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, methyl ester, (α Z)-MF C22 H33 F06 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (aZ)-, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, 2,2,2-trifluoroacetate (1:1) C24 H25 F2 N O8 S . C2 H F3 O2

MF

CM

Absolute stereochemistry. Double bond geometry as shown.

CM 2

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[2-[[4-(acetyloxy)-2-(3-fluoropheny1)-4-methyl-3-[4-(methylsulfony1)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]proylidene]-3-fluoro-, sodium salt (1:1)$
- MF C40 H38 F2 O10 S2 . Na

Na

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, $\alpha = [2-[3-[[(1,1-\dim thy)]]] - [4-(\min thy)]]$ methylbulfonyl)phenyl]ethylidene]-, methyl ester, $(\alpha 2)$ -MF C32 H38 07 S Si

^{**}PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT**

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-,
- (2S)-2-amino-3-ethoxy-3-oxopropyl ester
 MF C24 H25 F2 N O8 S

Absolute stereochemistry.

Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-,
 (22)-4-[(6-bromohexyl)oxy]-2-[4-(methylsulfonyl)phenyl]-4-oxo-3-phenyl-2buten-1-yl ester
- MF C30 H38 Br N O8 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[[6-
- (nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (aZ)-
- MF C25 H29 N O10 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 1H-Benzimidazole-4-carboxylic acid,

2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl)methyl]-, (22)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-vl ester

MF C43 H36 F2 N6 O7 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, (αZ)-
- MF C25 H28 N2 O12 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 1.3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[3-[[[(1,1dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αΕ)-C32 H38 O7 S Si

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-IN
- (aminosulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) MF C19 H18 F N O6 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, (αZ)MF C24 H25 F2 N O8 S
- CI COM

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester, sodium salt (1:1)
- MF C36 H32 O10 S2 . Na

Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

 10 Benzeneacetic acid, ac=[1-[4-(methylsulfonyl)]phenyl]-2-[[[3[(nitrooxy)methyl]phenoxy]carbonyl]oxy]ethylidene]-, methyl ester,
 (aZ)-
- MF C26 H23 N O10 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzenepropanoic acid, β -[(1-oxopropoxy)methyl]- α -phenyl-, ethyl ester
- MF C21 H24 O4

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Ethanaminium, 2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)

MF C24 H28 F2 N O6 S . Br

● Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, (α Z)-MF C25 H29 Br O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, ethyl ester, (α Z)-

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 1H-Benzimidazole-7-carboxylic acid, 2-ethoxy-1-[[2'-(2H-etrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, 3-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1oxo-2-buten-1-yl]oxy]-2-oxopropyl ester
- MF C46 H39 F N6 O10 S

PAGE 1-A

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, phenylmethyl ester, (α Z)-
- MF C28 H26 N2 O13 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[2-[[[3-(bromomethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, <math>(\alpha Z)$ -
- MF C26 H23 Br 07 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- TN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (aminosulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) MF C19 H17 F2 N 06 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L3
- Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-IN (methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N, N, N-trimethyl-MF C24 H29 F N O6 S
- COM

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneactic acid, a-[2-[[4-(acetyloxy)-2-(3,4-difluoropheny1)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-
- MF C36 H28 F4 O10 S2
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, 2-(diethylamino)ethyl$

ester, hydrochloride (1:1), (αZ)-C29 H38 N2 O10 S . C1 H

Double bond geometry as shown.

ME

HC1

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha [2-[4-[(22)-4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-1-oxobutoxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, <math>(\alpha Z)$ -
- MF C44 H44 F2 O12 S2
- CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- (methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester (9CI) MF C25 H30 F2 N2 O6 S

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4oxo-3-phenyl-2-buten-1-yl ester
- MF C25 H30 N2 09 S
- CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, $\alpha - [1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-(methylsulfonyl)phenyl]]$

1-oxohexyl]oxy]ethylidene]-, methyl ester, (αZ) -

F C24 H27 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, ~[2-(acetyloxy)-1-[4(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-,
(2S)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-3-ethoxy-3-oxopropyl ester,
(dZ)
MF C29 H33 F2 N 010 S

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (α Z)-
- MF C23 H24 N2 O13 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[[3-(hydroxymethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (α Z)-
- MF C26 H24 08 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[1-[4-(aminosulfony1)pheny1]-2-(benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI)$
- MF C24 H21 N 06 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-final content of the conte
- MF CZ4 HZ8 FZ N OE CI COM

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, 3-(3,4-difluorophenyl)-4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-[4-(methylsulfonyl)phenyl]-2-buten-1-yl ester C42 H44 F4 O9 S2 Si
- MF

$$\begin{array}{c} \text{Ne} \\ \text{t-Bu-Si-O} \\ \text{CH}_2 \\ \text{C-CH}_2 \\ \text{O-C-C-C-C} \\ \text{C-R} \end{array}$$

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-

(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (α Z)-MF C24 H27 N O10 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN INDEX NAME NOT YET ASSIGNED MF C44 H44 F2 O12 S2 . Na

Double bond geometry as shown.

Na

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α-[2-[(2S)-2-amino-3-hydroxy-1-oxopropoxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester (9CI) MF C22 H23 F2 N O7 S

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, 7-(nitrooxy)heptyl ester, (α Z)-MF C26 H31 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, methyl ester, (α Z)-

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Ethanaminium, 2-||(2Z)-4-(acetyloxy)-2-(3-fluoro
- IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1:1)
- MF C24 H29 F N O6 S . Br

Double bond geometry as shown.

● Br-

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha [2-[[[[4,5-$

bis(nitrooxy)pentyl]oxy|carbonyl]oxy]-1-[4- (methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (\alpha Z)- MF C25 H28 N2 013 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

Benzeneacetic acid, α-[2-[[3-[[(1,1dimethylathyl)dimethylsilyl]oxy]methyl]phenoxy]carbonyl]oxy]-1-[4(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (αZ)
MF C32 H38 08 S Si

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (aminosulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) MF C19 H19 N O6 S

Double bond geometry as shown.

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT **

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α =[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 1,6-hexanediyl ester, (α Z, α 'Z)- (9CI)
- MF C44 H46 O12 S2

Double bond geometry as shown.

$$\begin{array}{c} \text{Ne} & \text{Ph} & \text{Ph} \\ \text{Z} & \text{O} & \text{(CH2)6} \\ \text{AcO} & \text{OAc} \\ \end{array}$$

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha=[2-[[4-(acetyloxy]-2-(3,4-difluoropheny1)-3-[4-(methylsulfony1)pheny1]-1-oxo-2-buten-1-y1]oxy]-1-[4-(methylsulfony1)pheny1]ethylidene]-3,4-difluoro-, sodium salt (1:1)$
- MF C36 H28 F4 O10 S2 . Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha = [1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-$
- 1-oxohexyl]oxy]ethylidene]-, (1S)-1-carboxyethyl ester, (α Z)-MF C26 H29 N O11 S

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

TN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-4-[[(2R)-1-oxo-2-propylocty1]oxy]-2-buten-1-y1]oxy]-N,N,N-trimethy1-

C33 H46 F2 N O6 S ME

COM

Absolute stereochemistry.

Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN L-Aspartic acid, 4-[3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl] ester
- MF C23 H23 F2 N O8 S

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-

(methylsulfony1)phenyl]ethylidene]-, 5-(nitrooxy)pentyl ester, (αZ)-MF C24 H27 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[3-
- [(nitrooxy)methyl]benzoyl]oxy]ethylidene]-, methyl ester, (αZ)-MF C26 H23 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl-, bromide (1.1)
- MF C24 H28 F2 N O6 S . Br

Double bond geometry as shown.

• Br-

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[[[4,5-bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)penyl]ethylidene]-, methyl ester, (α Z)-MF C24 H26 N2 013 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α -[2-[[[(6-bromohexyl)oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (α Z)-

MF C26 H31 Br 07 S

Double bond geometry as shown.

**PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT **

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI)
 MF C20 H19 F O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

$$\begin{array}{c|c} \text{Me-} \\ \text{S} \\ \text{O} \\ \text{C} \\ \text{C}$$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, 2-(diethylamino)ethylester, (αZ) -
- MF C29 H38 N2 O10 S
- CI COM

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl ester, (αZ)-
- MF C30 H37 N O11 S

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, 3,4-difluoro- α -[1-[4-(methylsulfonyl)phenyl]-2-[(2R)-1-oxo-2-propyloctyl]oxy]ethylidene]-, methyl ester, (α Z)-MF C29 H36 F2 O6 S

Absolute stereochemistry.
Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, <math>(\alpha\mathbb{Z})-$
- MF C23 H24 N2 O12 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4-
- oxo-3-phenyl-2-butenyl ester, monohydrochloride (9CI) MF C25 H30 N2 O9 S . Cl H

Double bond geometry as shown.

HC1

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, \(\alpha\) - \((2 - (\acety\)) - 1 - [4 - (\amplitum \) \) (\amplitum \) (\amplitum

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[(2S)-2,6-diamino-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester, (αE) (9CI)
- MF C25 H30 F2 N2 O6 S

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha = [2-[[4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl$

 $3-[4-(\mathsf{methylsulfonyl})\mathsf{phenyl}]-1-\mathsf{oxo}-2-\mathsf{penten}-1-yl]\mathsf{oxy}]-2-\mathsf{methyl}-1-[4-(\mathsf{methylsulfonyl})\mathsf{phenyl}]\mathsf{propylidene}]-3-fluoro-$

MF C40 H38 F2 O10 S2

COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

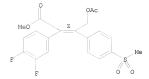
- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (αZ)-MF C24 H27 Br O7 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 84 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) MF C20 H18 F2 O6 S



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SINCE FILE TOTAL ENTRY SESSION 201.24 201.46

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ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

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E2 2 US2006-586567/AP

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1 --> US2006-586573/AP
E4
            0 US2006-586573/PRN
E5
                  US2006-586574/AP
            1
E6
                 US2006-586575/AP
US2006-586576/AP
            1
E7
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E8
            1
                 US2006-586577/AP
                 US2006-586578/AP
E9
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            1 US2006-586579/AP
1 US2006-586581/AP
E10
E11
E12
                 US2006-586583/AP
=> s us2006-586573/apps
             1 US2006-586573/AP
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0 US2006-586573/PRN 1.4 1 US2006-586573/APPS (US2006-586573/AP,PRN)

=> sel rn E1 THROUGH E34 ASSIGNED

=> file registry COST IN U.S. DOLLARS

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http://www.cas.org/support/stngen/stndoc/properties.html

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                  (10102-43-9/RN)
              1 108-24-7/BI
                  (108-24-7/RN)
              1 122-04-3/BI
                  (122-04-3/RN)
             1 14739-12-9/BI
                  (14739-12-9/RN)
             1 14739-15-2/BI
                  (14739-15-2/RN)
             1 14739-16-3/BI
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(14739-16-3/RN)

1 14739-18-5/BI (14739-18-5/RN)

1 14739-19-6/BI

(14739-19-6/RN)

1 162011-90-7/BI (162011-90-7/RN)

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(179174-76-6/RN)

1 179174-77-7/BI

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1 18343-90-3/BI

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1 861655-84-7/BI

(861655-84-7/RN)

1 861655-85-8/BI (861655-85-8/RN)

(861655-85-87RI

1 861655-86-9/BI

(861655-86-9/RN)

34 (10102-43-9/BI OR 108-24-7/BI OR 122-04-3/BI OR 14739-12-9/BI OR 14739-15-2/BI OR 14739-15-6/BI OR 14739-15-6/BI OR 1739-13-6-6/BI OR 1739-13-6-6/BI OR 162011-90-7/BI OR 179174-76-6/BI OR 179174-77-7/BI OR 179174-79-9/BI OR 18343-90-3/BI OR 3068-00-6/BI OR 329900-75-6/B I OR 329967-85-3/BI OR 50-78-2/BI OR 5048-26-0/BI OR 573-34-7/B

I OR 654068-92-5/BI OR 6835-50-3/BI OR 754242-03-0/BI OR 77-76-9 /BI OR 7761-88-8/BI OR 821-41-0/BI OR 849139-06-6/BI OR 861405-2 6-7/BI OR 861405-28-9/BI OR 861405-33-6/BI OR 861405-34-7/BI OR 861655-83-6/BI OR 861655-84-7/BI OR 861655-85-8/BI OR 861655-86-9/BI)

=> s 13 and 15 L6 4 L3 AND L5

=> d sca

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester, (αZ) -

MF C24 H26 N2 O12 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, (α 2)-
- MF C23 H24 N2 O12 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, (αZ)-

MF C25 H28 N2 O12 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L6 4 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, (<math>\alpha Z$)-
- MF C25 H28 N2 O12 S

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

2.40

209.76

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=> s 13

=> s 17 and (nitrosated or nitrosylated)

604 NITROSYLATED

1 L7 AND (NITROSATED OR NITROSYLATED)

=> d sca

L8

L8 1 ANSWERS ZCAPLUS COPYRIGHT 2009 ACS on STN

IC ICM A61K031-40

ICS A61K031-415; A61K031-421; A61K031-50; C07D207-325; C07D231-06; C07D237-14; C07D263-04; C07D263-06

CC 21-2 (General Organic Chemistry)

Section cross-reference(s): 1

II Preparation of nitrosated and nitrosylated

```
cyclooxygenase-2 inhibitors
cyclooxygenase 2 inhibitor nitrosated nitrosylated
prepn
Analgesics
Anti-inflammatory agents
   (preparation of nitrosated and nitrosylated
   cyclooxygenase-2 inhibitors)
Nitroso compounds
Nitrosvl complexes
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
   (preparation of nitrosated and nitrosylated
   cvclooxygenase-2 inhibitors)
329900-75-6, cyclooxygenase-2
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
(Biological study); PROC (Process)
   (mediated disorders; treatment; preparation of nitrosated and
   nitrosylated cyclooxygenase-2 inhibitors)
205580-05-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
   (preparation of nitrosated and nitrosylated
   cyclooxygenase-2 inhibitors)
                           346683-71-4P 346683-72-5P
346683-69-0P 346683-70-3P
                                                           346683-73-6P
              346683-76-9P
                             346683-77-0P
                                            346683-78-1P
                                                          346683-79-2P
346683-75-8P
346683-80-5P 346683-81-6P 346683-82-7P 346683-83-8P
346683-84-9P
              346683-85-0P 346683-86-1P 346683-87-2P 346683-88-3P
347162-90-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
   (preparation of nitrosated and nitrosylated
   cvclooxvgenase-2 inhibitors)
346683-99-6P
              346684-20-6P
                            346684-22-8P
RL: BYP (Byproduct); PREP (Preparation)
   (preparation of nitrosated and nitrosylated
   cvclooxygenase-2 inhibitors)
52-67-5, D-Penicillamine
                         53-86-1, Indomethacin
                                                  78-83-1.
2-Methyl-1-propanol, reactions 78-94-4, Methyl vinyl ketone, reactions
100-53-8, Benzyl mercaptan 627-18-9, 3-Bromo-1-propanol 1445-73-4,
1-Methyl-4-piperidone 1778-09-2, 4-Methylthioacetophenone 2417-72-3,
Methyl 4-bromomethylbenzoate
                             3446-89-7, 4-Methylthiobenzaldehyde
18162-48-6, tert-Butyldimethylsilyl chloride 21382-98-9,
4-Methylthiobenzonitrile 24214-73-1, Cyclohexylhydrazine hydrochloride
32047-53-3, 1-Amino-2-methyl-2-propanethiol hydrochloride 61040-78-6,
                               90878-19-6. Phenethylmagnesium chloride
2.4.6-Trimethoxybenzyl alcohol
194596-99-1
RL: RCT (Reactant); RACT (Reactant or reagent)
   (preparation of nitrosated and nitrosylated
   cvclooxygenase-2 inhibitors)
15581-80-3P
             28399-82-8P
                          40027-88-1P
                                         73303-88-5P.
2-Methyl-2-mercapto-1-propanol 86864-60-0P
                                             89031-84-5P
                                                           136881-95-3P
157672-00-9P
              170571-19-4P 170571-20-7P
                                            170571-71-8P
                                                          179174-91-5P
179174-92-6P
               179174-93-7P
                            179174-94-8P
                                            181695-72-7P
                                                          181695-81-8P
213764-17-1P
                                                          346683-90-7P
346683 - 91 - 8P 346683 - 92 - 9P 346683 - 94 - 1P 346683 - 95 - 2P 346683 - 96 - 3P
346683-97-4P 346683-98-5P 346684-00-2P 346684-01-3P 346684-02-4P
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346684-03-5P 346684-04-6P 346684-05-7P 346684-06-8P 346684-07-9P

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346684-08-0P 346684-09-1P 346684-10-4P 346684-11-5P 346684-12-6P
     346684-13-7P 346684-14-8P 346684-15-9P 346684-16-0P 346684-18-2P 346684-19-3P 346684-21-7P 347162-91-8P
                                                                346684-17-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
     346684-23-9P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of nitrosated and nitrosylated
        cyclooxygenase-2 inhibitors)
ALL ANSWERS HAVE BEEN SCANNED
=> s 17 and (nitrosated or nitrosylated or NO or (nitric (w) oxide))
          1340 NITROSATED
          604 NITROSYLATED
       3932570 NO
        220094 NOS
          2032 NOES
       4060112 NO
                 (NO OR NOS OR NOES)
        223122 NITRIC
             3 NITRICS
        223125 NITRIC
                 (NITRIC OR NITRICS)
       1991269 OXIDE
       377613 OXIDES
       2097881 OXIDE
                 (OXIDE OR OXIDES)
        131578 NITRIC (W) OXIDE
            11 L7 AND (NITROSATED OR NITROSYLATED OR NO OR (NITRIC (W) OXIDE))
=> d sca
     11 ANSWERS ZCAPLUS COPYRIGHT 2009 ACS on STN
     ICM C07C317-24
     ICS A61K031-21
INCL 514509000; 558482000
    25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
     Section cross-reference(s): 1
    Process for making nitric oxide releasing prodrugs of
    diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors
    nitric oxide releasing prodrug diphenylbutenoate hexyl
    nitrate
     Drug delivery systems
        (prodrugs; preparation of nitric oxide releasing
        prodrugs of diarv1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     329900-75-6, Cyclooxygenase 2
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (inhibitors; preparation of nitric oxide releasing
        prodrugs of diarv1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     10102-43-9, Nitric oxide, biological studies
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     64-19-7, Acetic acid, uses 67-68-5, Dmso, uses 68-12-2, Dmf, uses
     75-05-8, Acetonitrile, uses 75-09-2, Dichloromethane, uses 75-52-5,
     Nitromethane, uses 127-19-5, N,N-Dimethylacetamide
                                                           872-50-4,
     1-Methyl-2-pyrrolidinone, uses 1300-21-6, Dichloroethane 25321-22-6,
     Dichlorobenzene
```

1.9

L9

ΤТ

```
(preparation of nitric oxide releasing prodrugs of
        diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     937-14-4, m-Chloroperbenzoic acid 1504-58-1, 3-Phenyl-2-propyn-1-ol
     4286-55-9 7722-84-1, Hydrogen peroxide, reactions 10058-23-8,
     Potassium peroxymonosulfate
                                 11138-47-9, Sodium perborate
                                                                  74087-85-7,
                       78948-87-5, Magnesium monoperoxyphthalate
     Dimethyldioxirane
     210292-04-9, 4-Methylthiophenylmagnesium chloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of nitric oxide releasing prodrugs of
        diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     176594-44-8P
                   179174-79-9P 754242-10-9P 754242-11-0P
     754242-12-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     754241-98-0P
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
     study); PREP (Preparation); USES (Uses)
        (preparation of nitric oxide releasing prodrugs of
        diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0
=> d ibib hitstr 1-11
THE ESTIMATED COST FOR THIS REQUEST IS 42.79 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y) /N:v
   ANSWER 1 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:
                        2008:465556 ZCAPLUS
DOCUMENT NUMBER:
                         148:523285
TITLE:
                         Development of a discriminating in vitro dissolution
                        method for a poorly soluble NO-donating
                         selective cyclooxygenase-2 inhibitor
AUTHOR(S):
                         Papp, Robert; Luk, Pauline; Mullett, Wayne M.; Kwong,
                         Elizabeth; Debnath, Smita; Thibert, Roch
CORPORATE SOURCE:
                         Drug Metabolism and Pharmacokinetics, Merck Frosst
                        Center for Therapeutic Research, Kirkland, QC, H9H
                        3L1, Can.
SOURCE:
                        Journal of Pharmaceutical and Biomedical Analysis
                        (2008), 47(1), 16-22
                        CODEN: JPBADA; ISSN: 0731-7085
PUBLISHER:
                        Elsevier B.V.
DOCUMENT TYPE:
                        Journal
LANGUAGE:
                        English
     754241-98-0
     RL: PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (development of discriminating in vitro dissoln, method for poorly soluble
        NO-donating cyclooxygenase-2 inhibitor)
     754241-98-0 ZCAPLUS
RN
CN
     Benzeneacetic acid, a-[2-(acetyloxy)-1-[4-
     (methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (\alpha Z)-
     (CA INDEX NAME)
```

RL: NUU (Other use, unclassified); USES (Uses)

REFERENCE COUNT:

18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN 2006:495882 ZCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER:

145:14695

TITLE: Compounds for targeting mechanisms implicated in the

progression of stroke INVENTOR(S):

Munoz, Benito; Pavne, Joseph E.; Prasit, Petpiboon; Reger, Thomas S.; Smith, Nicholas D.; Stock, Nicholas

S.; McGuire, Angela R. Merck & Co., Inc., USA PATENT ASSIGNEE(S): PCT Int. Appl., 63 pp. SOURCE:

CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

KIND PATENT NO. DATE APPLICATION NO. DATE WO 2006055404 A2 20060526 WO 2005-US40851 20051110 WO 2006055404 A3 20060810 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN. YU. ZA. ZM. ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM PRIORITY APPLN. INFO.: US 2004-628280P P 20041116 OTHER SOURCE(S): MARPAT 145:14695

887908-51-2P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(compds. for targeting mechanisms implicated in progression of stroke) 887908-51-2 ZCAPLUS

1H-Benzimidazole-7-carboxylic acid,

2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-, 3-[[(2Z)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1oxo-2-buten-1-y1]oxy]-2-oxopropy1 ester (CA INDEX NAME)

PAGE 1-B

IT 887908-54-5 887908-56-7
RI: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (compds. for targeting mechanisms implicated in progression of stroke)

RN 887908-54-5 ZCAPLUS

CN 1H-Benzimidazole-4-carboxylic acid,
2-ethoxy-1-[[2'-(2H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]methyl]-,
(22)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2buten-1-yl ester (CA INDEX NAME)

RN 887908-56-7 ZCAPLUS

CN Ethanaminium, 2-[[(2Z)-2-(3,4-difluorophenyl)-4-[[(3,4-dihydro-6-hydroxy-2,5,7,8-tetramethyl-2H-1-benzopyran-2-yl)carbonyl]oxy]-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N, N, N-trimethyl- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT:

1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 3 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2006:383478 ZCAPLUS

DOCUMENT NUMBER: 144:432558

TITLE: Preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors.

INVENTOR(S): Munoz, Benito; Payne, Joseph Edward; Prasit,

Petpiboon; Reger, Thomas S.; Smith, Nicholas D.; Stock, Nicholas S.

PATENT ASSIGNEE(S): Merck & Co., Inc., USA SOURCE: PCT Int. Appl., 60 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patient. LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

DATEME	NO			ETNI		Da TE			2 DDI	TORT	TON	NIO.		D	a mrz			
PAIENI	PATENT NO.					KIND DATE					APPLICATION NO.							
NO 2006	WO 2006044230					2006	0427					20051007						
W0 2000				AM, AT, AU, AZ,														
w:																		
									DZ,									
									IS,									
									MA,									
									PL,									
					TJ,	TM,	TN,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,		
			ZM,															
RW:	ΑT,																	
									PΤ,									
									ML,									
							SD,	SL,	SZ,	ΤZ,	UG,	ZM,	ZW,	AM,	ΑZ,	BY,		
			MD,	RU,	ΤJ,	TM												
IORITY APP									US 2	004-	6179	62P		P 2	0041	012		
HER SOURCE	(S):			MARI	PAT	144:	4325	58										
885020-	33-7	P 88	5020	-34-	8P 8	8502	0-36	-0P										
885020-	37-1	P 88	5020	-38-	2P													
RL: PAC	(Ph	arma	colo	gica.	l ac	tivi	ty);	SPN	(Sy	nthe	tic ;	prep	arat	ion)	; TH	U		
(Therap	euti	c us	e); 1	BIOL	(Bi	olog	ical	stu	dy);	PRE	P (P	repa:	rati	on);	USE	S		
(Uses)						-												
(cla	imed	com	poun	d; p	repa	rati	on o	f me	thy1:	sulf	onyl	phen	ylal	keno	ates	as '		

soluble prodrugs of COX-2 inhibitors)

885020-33-7 ZCAPLUS RN

CN Ethanaminium, 2-[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N, N, N-trimethyl- (CA INDEX NAME)

Double bond geometry as shown.

RN 885020-34-8 ZCAPLUS

CN Ethanaminium, 2-[[(2Z)-4-(acetvloxv)-2-(3-fluorophenv1)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N,N,N-trimethyl- (CA INDEX NAME)

RN 885020-36-0 ZCAPLUS

CN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3, 4-difluoro-, (αZ) -, (2S)-2-amino-3-ethoxy-3-oxopropyl ester, 2,2,2-trifluoroacetate (1:1) (CA INDEX NAME)

CM 1

CRN 885020-35-9 CMF C24 H25 F2 N O8 S

Absolute stereochemistry. Double bond geometry as shown.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 885020-37-1 ZCAPLUS

CN L-Aspartic acid, 4-[(2Z)-3-(3,4-difluorophenyl)-4-ethoxy-2-[4-(methylsulfonyl)phenyl]-4-oxo-2-buten-1-yl] ester (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

- RN 885020-38-2 ZCAPLUS
- CN Benzeneacetic acid, α-[2-[[(2S)-2,6-diamino-1-oxohexyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, monoethyl ester, (κΕ)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry as shown.

IT 885020-42-8P 885020-43-9P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors)

- RN 885020-42-8 ZCAPLUS
- CN Ethanaminium, 2-[[(2Z)-4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)penyl)-1-oxo-2-buten-1-yl]oxy]-N, N, N-trimethyl-, bromide (1:1) (CA INDEX NAME)

Br -

RN 885020-43-9 ZCAPLUS

CN Ethanaminium, 2-[[(22)-4-(acetyloxy)-2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-N, N, N-trimethyl-, bromide (1:1) (CA INDEX NAME)

Double bond geometry as shown.

• Br-

IT 885020-47-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of methylsulfonylphenylalkenoates as water soluble prodrugs of COX-2 inhibitors)

RN 885020-47-3 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-,

(2S) = $2-[[(1,1-dimethylethoxy)carbonyl]amino] = 3-ethoxy = 3-oxopropyl ester, <math>(\alpha Z)$ = (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:1315893 ZCAPLUS

DOCUMENT NUMBER: 144:212486

TITLE: Synthesis of a NO-Releasing Prodrug of Rofecoxib

AUTHOR(S):

Engelhardt, F. Conrad; Shi, Yao-Jun; Cowden, Cameron J.; Conlon, David A.; Pipik, Brenda; Zhou, George;

McNamara, James M.; Dolling, Ulf-H.

CORPORATE SOURCE: Department of Process Research, Merck Company, Rahway,

NJ, 07065-0900, USA

SOURCE: Journal of Organic Chemistry (2006), 71(2), 480-491

CODEN: JOCEAH; ISSN: 0022-3263 PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 144:212486

ΙT 875783-67-8P

RL: BYP (Byproduct); PREP (Preparation)

(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-pheny1-2-propyn-1-ol)

RN 875783-67-8 ZCAPLUS

CN Benzeneacetic acid, $\alpha - [2-(acetyloxy)-1-[4-$

(methylsulfonyl)phenyl]ethylidene]-, 1,6-hexanediyl ester,

(αZ,α'Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

754242-04-1P

RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation) (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-pheny1-2-propyn-1-ol)

754242-04-1 ZCAPLUS RN

CN Benzeneacetic acid, $\alpha = [2-(acetyloxy)-1-[4-$ (methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, (α Z)- (CA INDEX NAME)

Double bond geometry as shown.

IT 754242-12-1P

CN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenv1-2-propvn-1-ol)

RN 754242-12-1 ZCAPLUS

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (α Z)-(CA INDEX NAME)

Double bond geometry as shown.

IT 754241-98-0P

RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-phenyl-2-propyn-1-ol)

RN 754241-98-0 ZCAPLUS CN Benzeneacetic acid.

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (αZ) -(CA INDEX NAME)

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

14

L9 ANSWER 5 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2005:963804 ZCAPLUS

DOCUMENT NUMBER: 143:266677

TITLE: Process for making nitric oxide

releasing prodrugs of diary1-2-(5H)-furanones as cvclooxygenase-2 inhibitors

INVENTOR(S): Shi, Yao-Jun; Engelhardt, F. Conrad; Cowden, Cameron

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS

John; Conlon, David A.; Pipik, Brenda

PATENT ASSIGNEE(S): USA

SOURCE: U.S. Pat. Appl. Publ., 16 pp.

CODEN: USXXCO DOCUMENT TYPE: Patent

LANGUAGE: English FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

REFERENCE COUNT:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
US 20050192346	A1	20050901	US 2005-66676	20050225		
PRIORITY APPLN. INFO.:			US 2004-549126P P	20040301		
OTHER SOURCE(S):	CASRE	EACT 143:266	677; MARPAT 143:266677			
IT 754242-12-1P						
RL: RCT (Reactant);	SPN	(Synthetic pr	reparation); PREP (Prepar	ation); RAC		
(Reactant or reagen	t)					
(preparation of	nitrio	c oxide relea	asing prodrugs of			
diary1-2-(5H)-fu	ranone	es as cycloo:	xygenase-2 inhibitors)			
RN 754242-12-1 ZCAPLU	S	-				

RN 754242-12-1 ZCAPLUS CN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (αZ)-(CA INDEX NAME)

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitric oxide releasing prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 754241-98-0 ZCAPLUS

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-CN

(methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (aZ)-(CA INDEX NAME)

Double bond geometry as shown.

ANSWER 6 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2005:696873 ZCAPLUS

DOCUMENT NUMBER: 143:172624

TITLE: Preparation of nitric oxide releasing prodrugs of diary1-2(5H)-furanones as

cyclooxygenase-2 inhibitors

Dufresne, Claude; Berthelette, Carl; Li, Lianhai; INVENTOR(S): Guay, Daniel; Gallant, Michel; Lacombe, Patrick;

Aspiotis, Renee; Wang, Zhaovin; Sturino, Claudio F. PATENT ASSIGNEE(S): Merck Frosst Canada & Co., Can.

SOURCE: PCT Int. Appl., 38 pp.

CODEN: PIXXD2 DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.							DATE				ICAT	DATE					
WO 2005070883																	
	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BW,	BY,	BZ,	CA,	CH,
		CN,	CO.	CR,	CU,	CZ,	DE,	DK.	DM,	DZ,	EC,	EE,	EG,	ES.	FI,	GB,	GD,
		GE,	GH,	GM,	HR.	HU,	ID,	IL.	IN.	IS,	JP,	KE.	KG,	KP,	KR.	KZ,	LC,
		LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NA,	NI,
		NO.	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,
		TJ,	TM.	TN.	TR.	TT.	TZ,	UA.	UG,	US,	UZ,	VC.	VN.	YU.	ZA.	ZM,	ZW
	RW:						MW,										
		AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,
		EE,	ES,	FI,	FR,	GB,	GR,	HU,	IE,	IS,	IT,	LT,	LU,	MC,	NL,	PL,	PT,
		RO,	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
		MR,	NE,	SN,	TD,	TG											
AU	2005	2062	28		A1		2005	0804		AU 2	005-	2062	28		2	0050	125
CA	2554	334			A1		2005	0804		CA 2	005-	2554	334		2	0050	125
EP	1711	459			A1		2006	1018		EP 2	005-	7064	13		2	0050	125
	R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
		IE,	SI,	LT,	LV,	FI,	RO,	CY,	TR,	BG,	CZ,	EE,	HU,	PL,	SK,	IS	
CN	1914	169			A		2007	0214		CN 2	005-	8000	3263		2	0050	125
JP	2007	5204	83		T		2007	0726		JP 2	006-		20050125				

US 20080242643 A1 20081002 US 2006-586381 20060718 IN 2006DN04347 20070713 IN 2006-DN4347 20060727 A PRIORITY APPLN. INFO.: US 2004-539666P P 20040127 WO 2005-CA83 W 20050125

CASREACT 143:172624; MARPAT 143:172624 OTHER SOURCE(S):

861430-33-3P 861430-34-4P 861430-36-6P

861430-38-8P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of nitric oxide releasing prodrugs of

diary1-2(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 861430-33-3 ZCAPLUS

CN Benzeneacetic acid, α -[2-[[[[4,5-

bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (aZ)- (CA INDEX NAME)

Double bond geometry as shown.

RN 861430-34-4 ZCAPLUS

CN Benzeneacetic acid, α -[2-[[[4,5bis(nitrooxy)pentyl]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, (aZ)- (CA INDEX NAME)

- RN 861430-36-6 ZCAPLUS
- CN Benzeneacetic acid, $\alpha=[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, <math>(\alpha Z)$ (CA INDEX NAME)

Double bond geometry as shown.

- RN 861430-38-8 ZCAPLUS
- CN Benzeneacetic acid, α -[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, phenylmethyl ester, (α Z)-(CA INDEX NAME)

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 7 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

2005:696865 ZCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 143:193802

TITLE: Preparation of nitric oxide

releasing prodrugs of diary1-2(5H)-furanones as cyclooxygenase-2 inhibitors

INVENTOR(S):

Berthelette, Carl; Li, Lianhai; Beaulieu, Christian; Wang, Zhaoyin; Sturino, Claudio F.

Merck Frosst Canada & Co., Can. PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 41 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1 PATENT INFORMATION:

PAT	PATENT NO.					KIND DATE					ICAT	DATE					
WO	2005	0708	74		A1 2005080								20050125				
	₩:										BG,						
											EC,						
											JP,						
											SC.						
											UZ,						
	RW:	BW,	GH,	GM,	KE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,
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											IT,						
							BF,	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,
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											CZ,						
	1914										2005-						
											2006-					0050: 0060:	
	2008										2006-						
PRIORITY					n		2007	0,13			2004-					0040	

OTHER SOURCE(S): CASREACT 143:193802; MARPAT 143:193802

IT 861655-83-6P 861655-84-7P 861655-85-8P

861655-86-9P

RL: ADV (Adverse effect, including toxicity); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL

(Biological study); PREP (Preparation); USES (Uses)
(preparation of nitric oxide releasing prodrugs of

diaryl-2(5H)-furanones as cyclooxygenase-2 inhibitors)

RN 861655-83-6 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5,6-bis(nitrooxy)hexyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

RN 861655-84-7 ZCAPLUS

CN Benzeneacetic acid, a-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (5R)-5,6-bis(nitrooxy)hexyl ester, (aZ)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

RN 861655-85-8 ZCAPLUS

CN Benzeneacetic acid, a-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 4,5-bis(nitrooxy)pentyl ester, (aZ)- (CA INDEX NAME)

861655-86-9 ZCAPLUS RN

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3,4-bis(nitrooxy)butyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 8 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2004:739958 ZCAPLUS DOCUMENT NUMBER: 141:260542

TITLE: Preparation of nitric oxide

releasing prodrugs of diary1-2-(5H)-furanones as

selective cvclooxvgenase-2 inhibitors

INVENTOR(S): Berthelette, Carl; Li, Lianhai; Sturino, Claudio;

Wang, Zhaoyin

PATENT ASSIGNEE(S): Merck Frosst Company, Can. SOURCE:

U.S. Pat. Appl. Publ., 19 pp.

CODEN: USXXCO Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

DOCUMENT TYPE:

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PATENT NO.	KIND	L	DATE			APPL	ILMI.	DATE						
		-												
US 2004017633	31	A1	2	20040	0909	1	US 2	004-	7902	88		2	0040	301
US 7169809		B2	2	2007	0130									
AU 2004240700	AU 2004240700 A1						AU 2	004-2	20040301					
CA 2517490	CA 2517490 A1					(CA 2	004-2	20040301					
WO 2004103955	WO 2004103955				1202	02 WO 2004-CA314						20040301		
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GE, C	GH, GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,
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         RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
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             ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
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             TD, TG
     EP 1601644
                          A1
                                20051207
                                            EP 2004-761562
                                                                    20040301
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                          В1
                                20090527
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     JP 2007516954
                          Т
                                20070628
                                            JP 2006-529472
                                                                    20040301
PRIORITY APPLN. INFO.:
                                            US 2003-452124P
                                                                   20030305
                                            WO 2004-CA314
                                                                 W 20040301
OTHER SOURCE(S):
                         MARPAT 141:260542
    754241-98-0P 754241-99-1P 754242-00-7P
     754242-01-8P 754242-02-9P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of nitric oxide releasing prodrugs of
        diarylfuranones as selective COX-2 inhibitors)
     754241-98-0 ZCAPLUS
RN
CN
     Benzeneacetic acid, a-[2-(acetyloxy)-1-[4-
     (methylsulfonyl)phenyl]ethylidene]-, 6-(nitrooxy)hexyl ester, (\alphaZ)-
     (CA INDEX NAME)
```

Double bond geometry as shown.

RN 754241-99-1 ZCAPLUS

CN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4oxo-3-phenyl-2-butenyl ester, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 754242-00-7 ZCAPLUS

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 5-(nitrooxy)pentyl ester, (α Z)-(CA INDEX NAME)

Double bond geometry as shown.

RN 754242-01-8 ZCAPLUS

CN Benzeneacetic acid, α =[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 7-(nitrooxy)heptyl ester, (α Z)-(CA INDEX NAME)

Double bond geometry as shown.

RN 754242-02-9 ZCAPLUS

CN Glycine, (2Z)-2-[4-(methylsulfonyl)phenyl]-4-[[6-(nitrooxy)hexyl]oxy]-4oxo-3-phenyl-2-buten-1-yl ester (CA INDEX NAME) Double bond geometry as shown.

IT 754242-04-1P 754242-08-5P 754242-09-6P

754242-12-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

RN 754242-04-1 ZCAPLUS

CN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-, 6-bromohexyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

RN 754242-08-5 ZCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (22)-4-[(6-bromohexyl)oxy]-2-[4-(methylsulfonyl)phenyl]-4-oxo-3-phenyl-2-buten-1-yl ester (CA INDEX NAME)

RN 754242-09-6 ZCAPLUS

CN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-, (22)-2-[4-(methylsulfonyl)phenyl]-4-[6-(nitrooxy)hexyl]oxy]-4-oxo-3phenyl-2-buten-1-yl ester (CA INDEX NAME)

Double bond geometry as shown.

RN 754242-12-1 ZCAPLUS

CN Benzeneacetic acid, α =[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 6-hydroxyhexyl ester, (α Z)-(CA INDEX NAME)

Double bond geometry as shown.

21

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L9 ANSWER 9 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:
                        2004:101124 ZCAPLUS
DOCUMENT NUMBER:
                         140:163574
TITLE:
                        Preparation of nitric oxide
                        releasing diary1-2-(5H)-furanone prodrugs as selective
                         cyclooxygenase-2 inhibitors for treatment inflammatory
                         diseases
INVENTOR(S):
                         Berthelette, Carl; Lachance, Nicholas; Li, Lianhai;
                         Sturing, Claudio; Wang, Zhaovin; Young, Robert N.;
                         Dufresne, Claude
PATENT ASSIGNEE(S):
                         Merck Frosst Canada & Co., Can.
SOURCE:
                         PCT Int. Appl., 129 pp.
                         CODEN: PIXXD2
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:
                                           APPLICATION NO.
     PATENT NO.
                        KIND DATE
                                                                  DATE
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                                           -----
                               20040205 WO 2003-CA1115
     WO 2004011421
                        A1
                                                                  20030724
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
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             PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR,
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         RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
     CA 2493082
                              20040205 CA 2003-2493082
                         A1
                                                                 20030724
     AU 2003252515
                               20040216
                                         AU 2003-252515
                          A1
                                                                  20030724
     EP 1527045
                         A1
                               20050504
                                          EP 2003-771010
                                                                  20030724
         R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     US 20050261245
                         A1 20051124
                                            US 2005-521075
                                                                   20050112
     US 7199154
                         B2
                               20070403
PRIORITY APPLN. INFO.:
                                            US 2002-398683P
                                                              P 20020726
                                            US 2002-435341P
                                                              P 20021220
                                            WO 2003-CA1115
                                                              W 20030724
OTHER SOURCE(S):
                        CASREACT 140:163574; MARPAT 140:163574
IT
    654069-14-4P
     RL: BYP (Byproduct); PREP (Preparation)
        (preparation of nitric oxide releasing diarylfuranone
        prodrugs as selective cyclooxygenase-2 inhibitors for treatment of
        inflammatory diseases)
RN
    654069-14-4 ZCAPLUS
```

Double bond geometry as shown.

NAME)

Benzeneacetic acid, α -[2-[[3-[[[(1,1-

dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (aE)- (CA INDEX

IT 654068-75-4P 654068-76-5P 654068-79-8P 654068-81-2P 654068-81-2P 654068-81-2P 654068-81-2P 654068-81-2P 654068-87-8P 654068-89-P 654068-99-09 654068-99-09 F654068-99-09 F654068-99-09 F654068-99-09 F654068-90-09 F654068-90-0

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitric oxide releasing diarylfuranone prodrugs as selective cyclooxygenase-2 inhibitors for treatment of inflammatory diseases)

RN 654068-75-4 ZCAPLUS

CN Benzeneacstic acid, $\alpha = \{1 - [4 - (methylsulfonyl)phenyl] - 2 - [3 - (nitrooxy)methyl]benzoyl]oxy]ethylidene]-, methyl ester, <math>(\alpha Z) - (CA \times MAME)$

Double bond geometry as shown.

RN 654068-76-5 ZCAPLUS

CN Benzeneacetic acid, $\alpha=\{1-\{4-(methylsulfonyl)phenyl\}-2-[\{4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, methyl ester, (<math>\alpha$ Z)- (CA INDEX NAME)

- RN 654068-79-8 ZCAPLUS
- CN Benzeneacetic acid, $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, methyl ester, (<math>\alpha Z$)- (CA INDEX NAME)

Double bond geometry as shown.

- RN 654068-81-2 ZCAPLUS
- CN Benzeneacetic acid, α =[1-[4-(methylsulfonyl)phenyl]-2-[[[4-(nitrooxy)butoxy]carbonyl]oxy]ethylidene]-, ethyl ester, (α Z)- (CA INDEX NAME)

- RN 654068-83-4 ZCAPLUS
- CN Benzeneacetic acid, $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (<math>\alpha$ Z)-

(CA INDEX NAME)

Double bond geometry as shown.

RN 654068-84-5 ZCAPLUS

CN Benzeneacetic acid, α =[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, ethyl ester, (α Z)-(CA INDEX NAME)

Double bond geometry as shown.

RN 654068-85-6 ZCAPLUS

CN Benzeneacetic acid, a-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, 2-(diethylamino)ethyl ester, (aZ)- (CA INDEX NAME)

- RN 654068-86-7 ZCAPLUS
- CN Benzeneacetic acid, a-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl ester, (aZ)- (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

- RN 654068-87-8 ZCAPLUS
- CN Benzeneacetic acid, a-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-1-oxohexyl]oxy]ethylidene]-, (1S)-1-carboxyethyl ester, (aZ)- (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry as shown.

- RN 654068-88-9 ZCAPLUS
- CN Benzeneacetic acid, a-[1-[4-(methylsulfonyl)phenyl]-2-[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, methyl ester, (α Z)-(CA INDEX NAME)

RN 654068-89-0 ZCAPLUS

CN Benzeneacetic acid, a=[1-[4-(methylsulfonyl)phenyl]-2-[[[5-(nitrooxy)pentyl)oxy]carbonyl]oxplethylidene]-, 2-(diethylamino)ethyl ester, hydrochloride (1:1), (a2)- (CA INDEX NAME)

Double bond geometry as shown.

HC1

RN 654068-90-3 ZCAPLUS

CN Benzeneacetic acid, a-[1-[4-(methylaulfonyl)phenyl]-2-[[[3-[(nitrooxy)methyl]phenoxy]carbonyl]oxy]ethylidene]-, methyl ester, (aZ)- (CA INDEX NAME)

- IT 654068-91-4P 654068-95-8P 654068-98-1P
 654069-03-1P 654069-03-P 654069-10-0P
 654069-11-1P 654069-15-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation of nitric oxide releasing diarylfuranone
 prodrugs as selective cyclooxygenase-2 inhibitors for treatment of
 inflammatory diseases)
 RN 654068-91-4 ZCAPLUS
- CN Benzeneacetic acid, α-[2-[[3-[[[(1,1-dimethylethyl)dimethylsilylloxylmethyl]ben

dimethylethyl)dimethylsilyl]oxy]methyl]benzoyl]oxy]-1-[4- (methylsulfonyl)phenyl]ethylidene]-, methyl ester, (α Z)- (CA INDEX NAME)

Double bond geometry as shown.

- RN 654068-95-8 ZCAPLUS
- CN Benzeneacetic acid, α =[2-[{(4-bromobutoxy)carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (α Z)- (CA INDEX NAME)

RN 654068-98-1 ZCAPLUS

CN Benzeneacetic acid, α-[2-[[(4-bromobutoxy)carbony1]oxy]-1-[4-(methylsulfony1)pheny1]ethylidene]-, ethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

RN 654069-03-1 ZCAPLUS

CN Benzeneacetic acid, $\alpha-[2-[[[(6-bromohexyl)oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, ethyl ester, <math>(\alpha Z)-$ (CA INDEX NAME)

Double bond geometry as shown.

RN 654069-09-7 ZCAPLUS

CN Benzeneacetic acid, $\alpha = [2 - [[[3 - [[[(1, 1 -$

 $\label{limits} $$ \dim thylsilyl[oxy] = honoxy[carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, $(\alpha Z)-$ (CA INDEX NAME)$ $$$

Double bond geometry as shown.

- RN 654069-10-0 ZCAPLUS
- CN Benzeneacetic acid, α -[2-[[[3-(hydroxymethyl)phenoxy]carbonyl]oxy]-1[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (α Z)- (CA
 INDEX NAME)

Double bond geometry as shown.

- RN 654069-11-1 ZCAPLUS
- CN Benzeneacetic acid, α -[2-[[[3-(bromomethyl)phenoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (α Z)- (CA INDEX NAME)

RN 654069-15-5 ZCAPLUS

CN Benzeneacetic acid, α -[2-[[3-(bromomethyl)benzoyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (\alpha Z)- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 10 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN ACCESSION NUMBER: 2001:472491 ZCAPLUS

DOCUMENT NUMBER: 135:76524

TITLE: Preparation of nitrosated and nitrosvlated cyclooxygenase-2 inhibitors

INVENTOR(S): Bandarage, Ramani R.; Bandarage, Upul K.; Fang,

Xinqin; Garvey, David S.; Letts, L. Gordon; Schroeder,

Joseph D.; Tam, Sang William Nitromed, Inc., USA PCT Int. Appl., 230 pp.

PATENT ASSIGNEE(S): SOURCE:

CODEN: PIXXD2 DOCUMENT TYPE:

Patent English

LANGUAGE: FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATE	KIND DATE			APPLICATION NO.						DATE									
						-													
WO 2001045703					A1 20010628			WO 2000-US35014							20001222				
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            SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN,
            YU, ZA, ZW
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                                        MX 2002-6312
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    US 20030220228
                              20031127
                                         US 2003-463671
                                                                20030618
    US 7166618
                              20070123
                       A1
B2
    US 20070060571
                              20070315
                                         US 2006-599519
                                                                20061115
                              20081007
    US 7432285
                       A1
                             20090416
    US 20090099139
                                          US 2008-196184
                                                                20080821
PRIORITY APPLN. INFO.:
                                          US 1999-171623P
                                                            P 19991223
                                          US 2000-226085P
                                                             P 20000818
                                          US 2000-741816
                                                            A3 20001222
                                          WO 2000-US35014
                                                            W 20001222
                                          US 2003-463671
                                                            A3 20030618
                                          US 2006-599519
                                                            A3 20061115
                       MARPAT 135:76524
    346683-81-6P 346683-83-8P
```

OTHER SOURCE(S):

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitrosated and nitrosylated

cyclooxygenase-2 inhibitors)

RN 346683-81-6 ZCAPLUS

CN Benzeneacetic acid, $\alpha - [2-(acetyloxy)-1-[4-$

(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 3-[4-[1-methvl-1-(nitrosothio)ethvl]-2-oxo-3-oxazolidinvl]propvl ester, (αZ)- (CA INDEX NAME)

RN 346683-83-8 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, 2-[1-methyl-4-(nitrosothio)-4-piperidinyl]ethyl ester, (αZ)- (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT:

4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 11 OF 11 ZCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:462317 ZCAPLUS

DOCUMENT NUMBER: 125:114294

ORIGINAL REFERENCE NO.: 125:21435a,21438a

TITLE: Preparation of stilbene derivatives useful as

cyclooxygenase-2 inhibitors

INVENTOR(S): Atkinson, Joseph G.; Wang, Zhaoyin PATENT ASSIGNEE(S): Merck Frosst Canada Inc., Can.

SOURCE: PCT Int. Appl., 80 pp.

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA	TENT	KIND DATE				APPLICATION NO.						DATE							
WO	9613			A1 19960509				WO :	1995-	CA60	19951024								
	W:	AL,	AM,	AU,	BB,	BG,	BR,	BY,	CA,	CN,	CZ,	EE,	FI,	GE,	HU,	IS,	JP,		
		KG,	KR,	KZ,	LK,	LR,	LT,	LV,	MD,	MG,	MK,	MN,	MX,	NO,	NZ,	PL,	RO,		
		RU,	SG,	SI,	SK,	TJ,	TM,	TT,	UA,	US,	, UZ								
	RW:	KE,	LS,	MW,	SD,	SZ,	UG,	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙE,		
		IT,	LU,	MC,	NL,	PT,	SE,	BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	ML,	MR,		
		NE,	SN,	TD,	TG														
CA	2200	462			A1 19960509					CA :	1995-	2200	19951024						
AU	AU 9536950					A 19960523				AU 1995-36950					19951024				
AU	6889	B2		1998	0319														
EP	EP 788476									EP 1995-944787					19951024				
EP	7884	B1	1999	1020															
						DK,	ES,	FR,	GB,	GR,	IE,	IT,	LI,	LU,	NL,	PT,	SE		
JP	1050	7765			T		1998	0728		JP :	1995-	5142	04		1	.9951	024		
AT	AT 185797						T 19991115						19951024						
ES	2139	959			Т3		2000	0216			1995-								
US	5849	943			A		1998	1215		US :	1997-	8171	28		1	.9970	407		
PRIORIT	Y APP	LN.	INFO	. :						US :	1994-	3301	72		A1 1	9941	027		
										WO :	1995-	CA60	1		W 1	.9951	024		
OTHER S	OURCE	(S):		MARPAT 125:11429				94											

ΙT 179174-84-6P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of stilbene derivs. useful as cyclooxygenase-2 inhibitors)

RN 179174-84-6 ZCAPLUS

Benzeneacetic acid, $\alpha - (2 - (acetvloxv) - 1 - (4 -$

(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

179174-89-1 179174-90-4 179174-95-9 179175-00-9 179175-04-3 179175-09-8

179175-14-5

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(preparation of stilbene derivs. useful as cyclooxygenase-2 inhibitors)

RN 179174-89-1 ZCAPLUS

Benzeneacetic acid, α -[2-(benzoyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

RN 179174-90-4 ZCAPLUS

CN Benzeneacetic acid, a-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179174-95-9 ZCAPLUS

CN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179175-00-9 ZCAPLUS

CN Benzeneacetic acid, $\alpha - \{2 - (acetyloxy) - 1 - \{4 - (aminosulfonyl)phenyl\}ethylidene] -, methyl ester, (Z) - (9CI) (CA INDEX NAME)$

RN 179175-04-3 ZCAPLUS
CN Benzeneacetic acid, a=[1-[4-(aminosulfonyl)phenyl]-2(benzoyloxy)ethylidene]-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179175-09-8 ZCAPLUS CN Benzeneacetic acid,

Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-3,4-difluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

RN 179175-14-5 ZCAPLUS

CN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(aminosulfonyl)phenyl]ethylidene]-4-fluoro-, methyl ester, (Z)- (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 10:54:15 ON 17 JUN 2009)

FILE 'REGISTRY' ENTERED AT 10:54:48 ON 17 JUN 2009

STRUCTURE UPLOADED

4 S SAM SSS L1 L2 L3 84 S FULL SSS L1

FILE 'ZCAPLUS' ENTERED AT 11:14:23 ON 17 JUN 2009

E US2006-586573/APPS

L4 1 S US2006-586573/APPS

SEL RN

FILE 'REGISTRY' ENTERED AT 11:15:49 ON 17 JUN 2009

34 S E1-E34 4 S L3 AND L5 L6

FILE 'ZCAPLUS' ENTERED AT 11:18:58 ON 17 JUN 2009

L7 18 S L3

L8 1 S L7 AND (NITROSATED OR NITROSYLATED)

L9 11 S L7 AND (NITROSATED OR NITROSYLATED OR NO OR (NITRIC (W) OXIDE

=> exit

ALL L# OUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

LOGOFF? (Y) /N/HOLD: y

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION FULL ESTIMATED COST 67.29 277.05

STN INTERNATIONAL LOGOFF AT 11:59:21 ON 17 JUN 2009

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:SSPTAVXR1614

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * *	* *	* *	* *	* Welcome to STN International * * * * * * * * * *										
NEWS	1			Web Page for STN Seminar Schedule - N. America										
NEWS		DEC	0.1	ChemPort single article sales feature unavailable										
NEWS		APR		CAS coverage of exemplified prophetic substances										
	-			enhanced										
NEWS		APR		STN is raising the limits on saved answers										
NEWS	5	APR	24	CA/CAplus now has more comprehensive patent assignee information										
NEWS	6	APR												
115110	7	APR	00	assignment/reassignment information CAS patent authority coverage expanded										
NEWS NEWS		APR		JAS patent authority coverage expanded ENCOMPLIT/ENCOMPLIT2 search fields enhanced										
NEWS		APR												
	-			Limits doubled for structure searching in CAS REGISTRY										
NEWS				STN Express, Version 8.4, now available										
NEWS		MAY		STN on the Web enhanced										
NEWS	12	MAY	11	BEILSTEIN substance information now available on										
				STN Easy										
NEWS	13	MAY	14	14 DGENE, PCTGEN and USGENE enhanced with increased limits for exact sequence match searches and										
				introduction of free HIT display format										
NEWS	14	MAY	15	INPADOCDB and INPAFAMDB enhanced with Chinese legal										
				status data										
NEWS	15	MAY	28	CAS databases on STN enhanced with NANO super role in										
				records back to 1992										
NEWS	16	JUN	01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN										
NEWS	17	JUN	26	NUTRACEUT and PHARMAML no longer updated										
NEWS	EXP	RESS		26 09 CURRENT WINDOWS VERSION IS V8.4,										
			AND	CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.										
NEWS	HOU	RS	ST	N Operating Hours Plus Help Desk Availability										
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agr	eeme	nt.	Thi	s agreement limits use to scientific research. Use										
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FILE 'REGISTRY' ENTERED AT 09:41:02 ON 29 JUN 2009 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ${\tt ZIC/VINITI}$ data file provided by InfoChem.

STRUCTURE FILE UPDATES: 28 JUN 2009 HIGHEST RN 1160218-33-6
DICTIONARY FILE UPDATES: 28 JUN 2009 HIGHEST RN 1160218-33-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2009.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

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, Q

chain nodes: 7 8 9 10 11 13 14 15 16 17 24 ring nodes:

```
1 2 3 4 5 6 12 18 19 20 21 22 25 26 27 28 29 30
chain bonds :
6-7 7-8 7-11 8-9 9-10 10-15 11-12 11-13 13-14 13-16 16-17
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-22 18-19 19-20 20-21 21-22 25-26
25-30 26-27 27-28 28-29 29-30
exact/norm bonds :
7-11 8-9 9-10 10-15 13-14 13-16 16-17
exact bonds :
6-7 7-8 11-12 11-13
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 12-18 12-22 18-19 19-20 20-21 21-22 25-26
25-30 26-27 27-28 28-29 29-30
isolated ring systems :
containing 1 : 12 :
G1:H,[*1],[*2]
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:CLASS 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:Atom
19:Atom 20:Atom 21:Atom 22:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom
L1
             STRUCTURE UPLOADED
=> d 11
L1 HAS NO ANSWERS
L1
                          STR
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *
Structure attributes must be viewed using STN Express query preparation.
=> s sam 11
SAMPLE SEARCH INITIATED 09:41:37 FILE 'REGISTRY'
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                                                                29 TO ITERATE
100.0% PROCESSED
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                                                                                                             3 ANSWERS
SEARCH TIME: 00.00.01
FULL FILE PROJECTIONS: ONLINE **COMPLETE**
                                        BATCH **COMPLETE**
PROJECTED ITERATIONS:
                                                    257 TO
                                                                        903
PROJECTED ANSWERS:
                                                      3 TO
                                                                        163
L2
                       3 SEA SSS SAM L1
=> d sca
        3 ANSWERS
                          REGISTRY COPYRIGHT 2009 ACS on STN
ΤN
        Benzeneacetic acid, \alpha = [2 - [4 - (acetyloxy) - 2 - (3 - fluorophenyl) - 4 - methyl-
        3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-methylsulfonyl)phenyl
```

(methylsulfonyl)phenyl]propylidene]-3-fluoro-

C40 H38 F2 O10 S2

MF C40

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, 3,4-difluoro- α -[1-[4-(methylsulfonyl)phenyl]-2-[(1-oxo-2-propyloctyl)oxy]ethylidene]-, (α Z)-
- MF C28 H34 F2 06 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L2 3 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- MF C40 H38 F2 O10 S2 . Na

Na

ALL ANSWERS HAVE BEEN SCANNED

=> s full sss 11
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 185.40 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 09:42:32 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 767 TO ITERATE

100.0% PROCESSED 767 ITERATIONS SEARCH TIME: 00.00.01 51 ANSWERS

L3 51 SEA SSS FUL L1

=> d sca

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Butanedioic acid, 1,4-bis[3-carboxy-3-(3-fluoropheny1)-1,1-dimethy1-2-[4-(methylsulfony1)pheny1]-2-propen-1-y1] ester
- MF C42 H40 F2 O12 S2
- CI COM

PAGE 2-A

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (aminosulfonyl)phenyl]ethylidene]-, (Z)- (9CI) MF C18 H17 N O6 S

ME CIO HI / N OO S

$$\begin{array}{c} \text{OAc} \\ \text{Z} \\ \text{CO}_2\text{H} \\ \text{Ph} \\ \end{array}$$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 3-Pyridinecarboxylic acid, 3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2-propen-1-yl ester, hydrochloride (1:1) MF C23 H17 F2 N O6 S. C.1 H

● HCl

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[[6-(nitrooxy)hexyl]oxy]carbonyl]oxy]ethylidene]-, (<math>\alpha$ Z)-
- MF C24 H27 N O10 S

$$\begin{array}{c} \text{O} \\ \text{O} \\ \text{O} \\ \text{Z} \\ \text{CO}_2\text{H} \\ \text{Ph} \\ \text{O} \\ \text{O} \\ \text{O} \end{array}$$

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 3-Pyridinecarboxylic acid, (2Z)-3-carboxy-3-(3,4-difluorophenyl)-2-[4-
- (methylsulfonyl)phenyl]-2-propen-1-yl ester MF C23 H17 F2 N O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, α-[2-(acetvloxy)-1-[4-
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylthio)phenyl]ethylidene]-, magnesium salt, hydrate (2:1:?),
- MF C19 H18 O4 S . x H2 O . 1/2 Mg

- ●1/2 Mg
 - ●x H2O

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN L-Proline, N-[(1S)-2-ethoxy-1-(2-phenylethyl)-2-propenyl]-L-alanyl-, (2Z)-3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2-
- propenyl ester (9CI) MF C38 H42 F2 N2 O8 S

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester, sodium salt (1:1)
- MF C36 H32 O10 S2 . Na

Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, a-[2-[4-[[(22)-4-(acetyloxy)-2-(3-fluorophenyl)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-y1]oxy]-1-oxobutoxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-3-fluoro-, (aZ)-
- MF C44 H44 F2 O12 S2
- CI COM

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-, 3-czhoxy-2-[4-(methylsulfonyl)phenyl]-3-ph

3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester

MF C36 H32 010 S2

I COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-

(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, sodium salt, (Z)- (9CI)
MF C19 H16 F2 O6 S . Na

Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, α-[2-[[[4,5-bis(nitrooxy)penty]]oxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (αZ)MF C23 H24 N2 O13 S

MF C23 H24 N2 013 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (aminosulfonyl)phenyl]ethylidene]-3,4-difluoro-, (Z)- (9CI) ME C18 H15 F2 N 06 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Valeric acid, α, γ, δ -trihydroxy- α, β, δ triphenyl-, tribenzoate (2CI) C44 H34 O8
- MF

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[2-[[[(6-bromohexy1)oxy]carbony1]oxy]-1-[4-(methylsulfony1)pheny1]ethylidene]-, (<math>\alpha Z$)-
- MF C24 H27 Br 07 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN L-Aspartic acid, N-[(1,1-dimethylethoxy)carbonyl]-,
 4-[(22)-3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2propen-1-yl] 1-(1,1-dimethylethyl) ester
- MF C30 H35 F2 N O10 S

Absolute stereochemistry. Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, sodium salt (1:1) MF
 - C36 H28 F4 O10 S2 . Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- Benzeneacetic acid, 3,4-difluoro- α -[1-[4-(methylsulfonyl)phenyl]-2-IN [(1-oxo-2-propyloctyl)oxy]ethylidene]-, (aZ)-

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 2-Butenedioic acid, bis[3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propenyl] ester, disodium salt (9CI)
- MF C38 H32 O12 S2 . 2 Na

●2 Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN INDEX NAME NOT YET ASSIGNED
- MF C23 H25 Br 07 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 2-Butenedioic acid, bis[3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propenyl] ester (9CI)
- MF C38 H32 O12 S2
- CI COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-4-fluoro-, (αZ)-
- MF C19 H17 F 06 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-[[(2S)-2-amino-5-[(aminoiminomethyl)amino]-1-oxopentyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3, 4-difluoro-(9CI)
- MF C23 H26 F2 N4 O6 S

Absolute stereochemistry. Double bond geometry unknown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha-[1-[4-(methylsulfonyl)phenyl]-2-[[6-(nitrooxy)-$
 - 1-oxohexyl]oxy]ethylidene]-, (\alpha Z)-
- MF C23 H25 N O9 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN

IN Benzeneacetic acid, \(\alpha = [2 - (acetyloxy) - 2 - methyl - 1 - [4 - (methyl sulfonyl) phenyl] propylidene] - 3 - fluoro - , \((\alpha Z) - \)

MF C21 H21 F O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Glycine, N-[(1,1-dimethylethoxy)carbonyl]-,
 (2Z)-3-carboxy-2-[4-(methylsulfonyl)phenyl]-3-phenyl-2-propen-1-yl ester
 MF C24 H27 N 08 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 1H-Indole-2-carboxylic acid, 4,6-dichloro-3-[(1E)-3-oxo-3-(phenylamino)-1-propen-1-yl]-, (2Z)-3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2-propen-1-yl ester

MF C35 H24 C12 F2 N2 O7 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN L3
- Benzeneacetic acid, α -[2-[[4-(acetyloxy)-2-(3,4-difluorophenyl)-3-[4-IN (methylsulfonyl)phenyl]-1-oxo-2-buten-1-yl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-
- MF
- C36 H28 F4 O10 S2 CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN INDEX NAME NOT YET ASSIGNED
- MF C44 H44 F2 O12 S2 . Na

Double bond geometry as shown.

Na

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, 3-fluoro- α -[2-[4-[[2-(3-fluorophenyl)-3-[4-(methylsulfonyl)phenyl]-1,6-dioxo-2-hepten-1-yl]oxyl-1-oxobutoxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propylidene]-, sodium salt (1:1)
- MF C43 H42 F2 O11 S2 . Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (α Z)-
- MF C19 H16 F2 O6 S
- CI COM

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, 3-fluoro-ac/2-[4-[(2-(3-fluoropheny1)-3-[4-(methylsulfony1)pheny1]-1,6-dioxo-2-hepten-1-y1]oxy]-1-oxobutoxy]-2-methy1-1-(4-(methylsulfony1)pheny1)propylidene]-
- MF C43 H42 F2 O11 S2
- CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha = [1 [4 (aminosulfonyl)phenyl] 2 -$
- (benzoyloxy)ethylidene]-, (Z)- (9CI)

MF C23 H19 N O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN 3-Pyridinecarboxylic acid, 3-carboxy-3-(3,4-difluorophenyl)-2-[4-(methylsulfonyl)phenyl]-2-propen-1-yl ester
- MF C23 H17 F2 N O6 S
- CI COM

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[(4-bromobutoxy)carbonyl]oxy]-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-, (αZ)-MF C22 H23 Br O7 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (methylsulfonyl)phenyl]ethylidene]-3-fluoro-, (αZ)-MF C19 H17 F O6 S

... 025 112 2 00 0

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylthio)phenyl]ethylidene]-, (αZ) -
- MF C19 H18 O4 S
- CI COM

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, 3,4-difluoro-α-[1-[4-(methylsulfonyl)phenyl]-2-
- [[(2R)-1-oxo-2-propyloctyl]oxy]ethylidene]-, (αZ) -MF C28 H34 F2 O6 S
- ... 020 12 00 0

Absolute stereochemistry.
Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, $\alpha=[2-[\{4-(acetyloxy)-2-(3-fluoropheny1)-4-methyl-3-[4-(methylsulfony1)pheny1]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfony1)pheny1]propylidene]-3-fluoro-, sodium salt (1:1)$
- MF C40 H38 F2 O10 S2 . Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(2-methyl-1-oxopropoxy)-1-[4-(methylthio)phenyl]ethylidene]-, (α Z)-
- MF C21 H22 O4 S

$$\begin{array}{c} O & Pr-i \\ O & O \\ Z & CO_2H \\ \end{array}$$
 MeS

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- Benzeneacetic acid, $\alpha=[2-[14-(acetyloxy)-2-(3-fluoropheny1)-4-methyl-3-[4-(methylsulfonyl)phenyl]-1-oxo-2-penten-1-yl]oxy]-2-methyl-1-[4-(methylsulfonyl)phenyl]propyl[dene]-3-fluoro-$ IN
- C40 H38 F2 O10 S2 MF
- COM

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN Benzeneacetic acid, α -[2-(benzovloxv)-1-[4-IN (methylsulfonyl)phenyl]ethylidene]-, (Z)- (9CI) C24 H20 O6 S
- Double bond geometry as shown.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-[[[2,3-bis(nitrooxy)propoxy]carbonyl]oxy]-1-[4-(methylsulfonyl)phenyl]ethylidene]-, (αZ) -
- MF C21 H20 N2 O13 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α-[2-(acetyloxy)-1-[4-
- (aminosulfonyl)phenyl]ethylidene]-4-fluoro-, (Z)- (9CI)
- MF C18 H16 F N 06 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-
- (methylthio)phenyl]ethylidene]-, magnesium salt (2:1), (α Z)-C19 H18 O4 S . 1/2 Mg MF

Double bond geometry as shown.

●1/2 Mg

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- 1.3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- TN Benzeneacetic acid, α -[1-[4-(methylsulfonyl)phenyl]-2-[[[[5-(nitrooxy)pentyl]oxy]carbonyl]oxy]ethylidene]-, (aZ)-

C23 H25 N O10 S MF

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN Benzeneacetic acid, α -[2-[[(2S)-2,6-bis[[(1,1-IN dimethylethoxy)carbonyllaminol-1-oxohexylloxyl-1-[4-(methylsulfonyl)phenyl]ethylidene]-3,4-difluoro-, (aZ)- (9CI) C33 H42 F2 N2 O10 S

Absolute stereochemistry. Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-(methylsulfonvl)phenyl]ethylidene]-3,4-difluoro-
- C19 H16 F2 O6 S

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, α -[2-(acetyloxy)-1-[4-[(chloromethyl)sulfonyl]phenyl]ethylidene]-, (α Z)-
- MF C19 H17 C1 O6 S

Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN
- IN Butanedioic acid, 1,4-bis[3-carboxy-3-(3-fluorophenyl)-1,1-dimethyl-2-[4-(methylsulfonyl)phenyl]-2-propen-1-yl] ester, sodium salt (1:2)
- MF C42 H40 F2 O12 S2 . 2 Na

PAGE 2-A

●2 Na

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

- L3 51 ANSWERS REGISTRY COPYRIGHT 2009 ACS on STN IN Benzeneacetic acid, $\alpha [2-(acetyloxy)-1-[4-$
- (methylsulfonyl)phenyl]ethylidene]-, (αZ) -MF C19 H18 O6 S

ALL ANSWERS HAVE BEEN SCANNED

=> 1

1 IS NOT A RECOGNIZED COMMAND

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=> file zcaplus

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FULL ESTIMATED COST

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USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2009

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This file contains CAS Registry Numbers for easy and accurate substance identification.

```
=> s 13
T. 4
           15 L3
=> s 14 and (nitric (w) oxide)
        223611 NITRIC
             3 NITRICS
        223614 NITRIC
                 (NITRIC OR NITRICS)
       1994871 OXIDE
       378099 OXIDES
       2101601 OXIDE
                 (OXIDE OR OXIDES)
        131834 NITRIC (W) OXIDE
1.5
             7 L4 AND (NITRIC (W) OXIDE)
=> d sca
      7 ANSWERS ZCAPLUS COPYRIGHT 2009 ACS on STN
     ICM C07C317-24
     ICS A61K031-21
INCL 514509000; 558482000
     25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
     Section cross-reference(s): 1
     Process for making nitric oxide releasing prodrugs of
     diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors
     nitric oxide releasing prodrug diphenylbutenoate hexyl
     nitrate
     Drug delivery systems
        (prodrugs; preparation of nitric oxide releasing
        prodrugs of diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     329900-75-6, Cyclooxygenase 2
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (inhibitors; preparation of nitric oxide releasing
        prodrugs of diaryl-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     10102-43-9, Nitric oxide, biological studies
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (preparation of nitric oxide releasing prodrugs of
        diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     64-19-7, Acetic acid, uses 67-68-5, Dmso, uses
                                                       68-12-2, Dmf, uses
     75-05-8, Acetonitrile, uses 75-09-2, Dichloromethane, uses 75-52-5,
     Nitromethane, uses
                        127-19-5, N.N-Dimethylacetamide
                                                           872-50-4,
     1-Methyl-2-pyrrolidinone, uses
                                    1300-21-6, Dichloroethane 25321-22-6,
     Dichlorobenzene
     RL: NUU (Other use, unclassified); USES (Uses)
        (preparation of nitric oxide releasing prodrugs of
        diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     937-14-4, m-Chloroperbenzoic acid
                                        1504-58-1, 3-Phenv1-2-propvn-1-ol
                 7722-84-1, Hydrogen peroxide, reactions
     4286-55-9
                                                          10058-23-8,
     Potassium peroxymonosulfate
                                 11138-47-9, Sodium perborate
                                                                  74087-85-7.
                       78948-87-5, Magnesium monoperoxyphthalate
     Dimet.hvldioxirane
     210292-04-9, 4-Methylthiophenylmagnesium chloride
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of nitric oxide releasing prodrugs of
        diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     176594-44-8P 179174-79-9P 754242-10-9P
     754242-11-0P
                   754242-12-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of nitric oxide releasing prodrugs of
        diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)
     754241-98-0P
     RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
```

study); PREP (Preparation); USES (Uses) (preparation of nitric oxide releasing prodrugs of diary1-2-(5H)-furanones as cyclooxygenase-2 inhibitors)

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

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ICM A61K031-66

ICS A61K031-655; A61K031-21

INCL 514114000; X51-450.9; X51-415.1; X55-2 .1; X55-819.0; X55-848.2

27-6 (Heterocyclic Compounds (One Hetero Atom)) Section cross-reference(s): 1

TΙ Preparation of nitric oxide releasing prodrugs of

diary1-2-(5H)-furanones as selective cyclooxygenase-2 inhibitors

ST diarylfuranone prepn Rofecoxib prodrug nitric oxide; cyclooxygenase COX2 inhibitor diarylfuranone prepn prodrug nitric

oxide

ΙT Pain

(chronic, treatment of; preparation of nitric oxide

releasing prodrugs of diarylfuranones as selective COX-2 inhibitors) Anti-inflammatory agents

(nonsteroidal, medicaments with; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

Drug delivery systems

(oral; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

Analgesics

Anticoagulants

Antirheumatic agents

Combination chemotherapy

Human

(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

Drug delivery systems

(prodrugs; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

Inflammation

Osteoarthritis

Rheumatoid arthritis

(treatment of; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors) 50-78-2, Aspirin

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses) (medicaments with; preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

329967-85-3, Cyclooxygenase-1 329900-75-6, Cvclooxygenase-2 RL: BSU (Biological study, unclassified); BIOL (Biological study) (preparation of nitric oxide releasing prodrugs of

754241-98-0P 754241-99-1P 754242-00-7P 754242-01-8P 754242-02-9P RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of nitric oxide releasing prodrugs of diarylfuranones as selective COX-2 inhibitors)

diarylfuranones as selective COX-2 inhibitors)

108-24-7, Acetic anhydride 124-38-9, Carbondioxide, reactions 629-03-8, 1,6-Dibromohexane 1504-58-1, 3-Pheny1-2-propyn-1-o1 4286-55-9 4530-20-5, Boc-glycine 7697-37-2, Nitric acid, reactions 7722-84-1, Hydrogen peroxide, reactions 7761-88-8, Nitric acid silver(1+) salt, reactions 18162-48-6, tert-Butyl(dimethyl)silyl

```
RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of nitric oxide releasing prodrugs of
        diarylfuranones as selective COX-2 inhibitors)
     179174-76-6P, (2Z)-2-[4-(Methylsulfonyl)phenyl]-3-phenylbut-2-ene-1,4-diol
     179174-77-7P 179174-79-9P 654068-92-5P
                                               754242-03-0P
                                  754242-06-3P 754242-07-4P
                   754242-05-2P
     754242-04-1P
     754242-08-5P
                  754242-09-6P 754242-10-9P 754242-11-0P
     754242-12-1P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (preparation of nitric oxide releasing prodrugs of
        diarylfuranones as selective COX-2 inhibitors)
     10102-43-9, Nitric oxide, biological studies
     RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
        (preparation of nitric oxide releasing prodrugs of
        diarylfuranones as selective COX-2 inhibitors)
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1
      7 ANSWERS ZCAPLUS COPYRIGHT 2009 ACS on STN
L5
     25-8 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
TI
     Synthesis of a NO-Releasing Prodrug of Rofecoxib
ST
     nitric oxide releasing prodrug of rofecoxib;
     stereoselective carbometalation propargyl alc
     Metalation
        (carbometalation; stereoselective synthesis of a NO-releasing prodrug
        of rofecoxib including carbometalation reaction of propargyl alc.
        derivative)
     Stereoselective synthesis
        (stereoselective synthesis of a NO-releasing prodrug of rofecoxib
        including carbometalation reaction of propargyl alc. derivative)
     100-68-5P, Thioanisole
                            13205-48-6P, 4-Methylthiobenzoic acid
     162012-30-8P
                   875783-62-3P
                                  875783-63-4P
                                                 875783-67-8P
     RL: BYP (Byproduct); PREP (Preparation)
        (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps
        from 3-phenyl-2-propyn-1-ol)
     754242-04-1P
     RL: BYP (Byproduct); SPN (Synthetic preparation); PREP (Preparation)
        (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps
        from 3-phenv1-2-propvn-1-ol)
     10102-43-9, Nitric oxide, miscellaneous
     RL: MSC (Miscellaneous)
        (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps
        from 3-phenyl-2-propyn-1-ol)
     162011-90-7, Rofecoxib
     RL: PNU (Preparation, unclassified)
        (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps
        from 3-phenv1-2-propvn-1-ol)
     123-09-1
               1504-58-1, 3-Phenyl-2-propyn-1-ol
                                                  4286-55-9.
     6-Bromo-1-hexanol
                        176594-44-8
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps
        from 3-phenyl-2-propyn-1-ol)
                   210292-04-9P 754242-11-0P 754242-12-1P
     179174-79-9P
                   875783-64-5P 875783-65-6P 875783-66-7P
     875783-61-2P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps
```

chloride

162011-90-7 210292-04-9

from 3-phenyl-2-propyn-1-ol)

RL: SPN (Synthetic preparation); PREP (Preparation)

754241-98-0P

(synthesis of a NO-releasing prodrug of rofecoxib in five chemical steps from 3-pheny1-2-propyn-1-o1)

> TOTAL ENTRY SESSION 5 80 196 22

196.22

5.80

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d his

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FILE 'REGISTRY' ENTERED AT 09:41:02 ON 29 JUN 2009

L1 STRUCTURE UPLOADED

L2 3 S SAM L1

L3 51 S FULL SSS L1

FILE 'ZCAPLUS' ENTERED AT 09:46:45 ON 29 JUN 2009

T. 4 15 S L3 L5 7 S L4 AND (NITRIC (W) OXIDE)

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